



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 01:33 PM EDT

PDB ID : 3EYM  
Title : Structure of Influenza Haemagglutinin in complex with an inhibitor of membrane fusion  
Authors : Russell, R.J.; Kerry, P.S.; Stevens, D.A.; Steinhauer, D.A.; Martin, S.R.; Gambelin, S.J.; Skehel, J.J.  
Deposited on : 2008-10-21  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

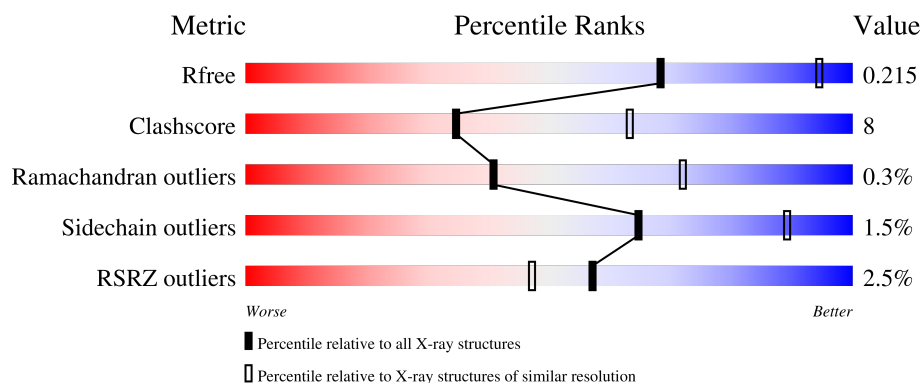
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


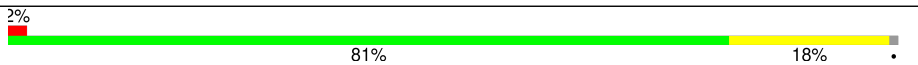

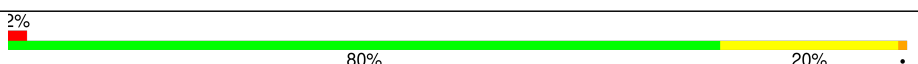
The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	
1	C	321	
1	E	321	
2	B	172	
2	D	172	

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Mol	Chain	Length	Quality of chain
2	F	172	<div><div></div><div>2%85%13%..</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11580 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

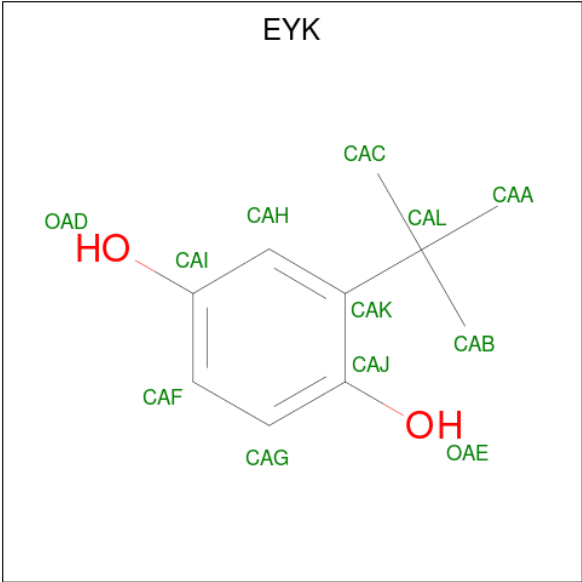
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2446	1532	429	472	13			
1	C	318	Total	C	N	O	S	0	0	0
			2455	1538	431	473	13			
1	E	318	Total	C	N	O	S	0	0	0
			2455	1538	431	473	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1399	868	246	279	6			
2	D	172	Total	C	N	O	S	0	0	0
			1390	868	246	270	6			
2	F	172	Total	C	N	O	S	0	0	0
			1399	868	246	279	6			

- Molecule 3 is 2-tert-butylbenzene-1,4-diol (three-letter code: EYK) (formula: C<sub>10</sub>H<sub>14</sub>O<sub>2</sub>).

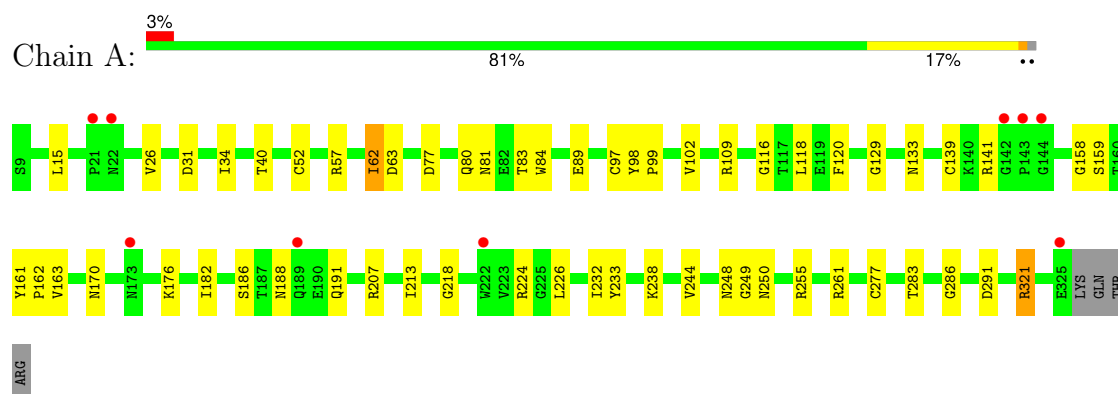


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			12	10	2		
3	D	1	Total	C	O	0	0
			12	10	2		
3	F	1	Total	C	O	0	0
			12	10	2		

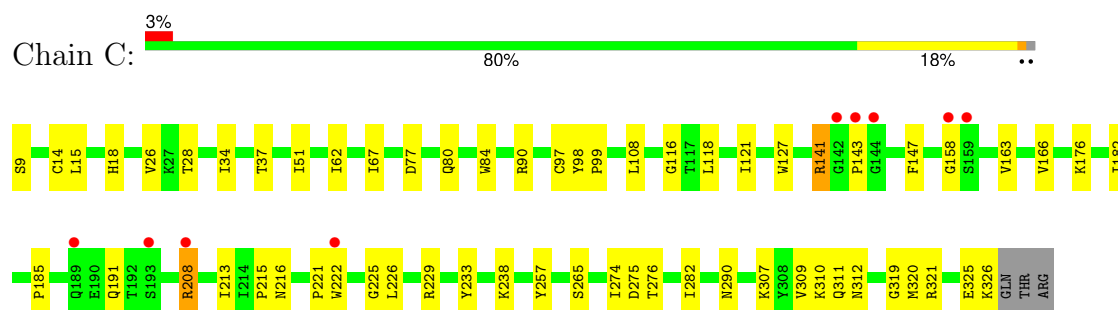
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

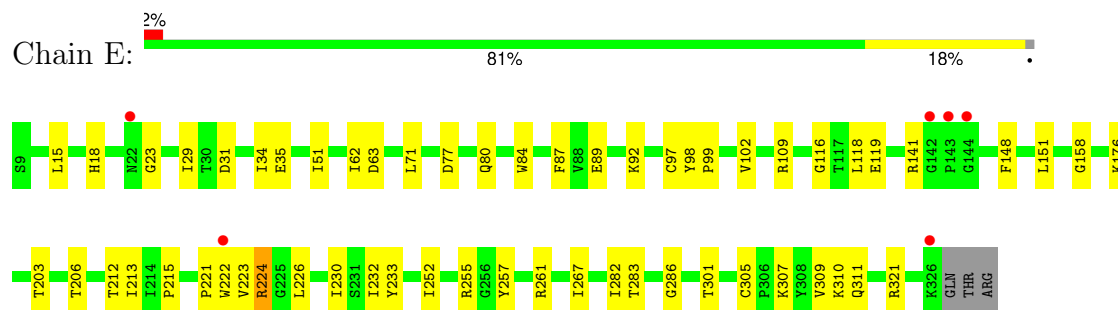
- Molecule 1: Hemagglutinin HA1 chain



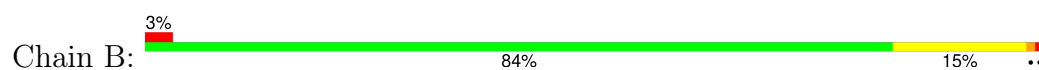
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

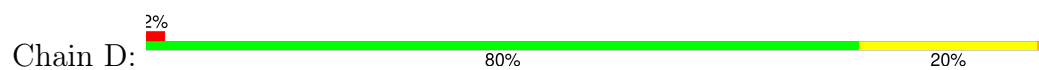


- Molecule 2: Hemagglutinin HA2 chain



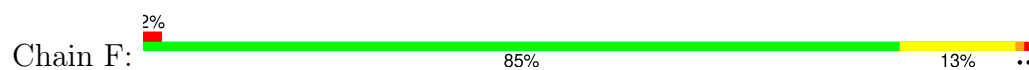


• Molecule 2: Hemagglutinin HA2 chain



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• Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.47Å 160.46Å 176.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.93-2.80) 100.0 (19.93-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.217 0.205 , 0.215	Depositor DCC
$R_{free}$ test set	5462 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EYK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.64	2/2502 (0.1%)	0.68	2/3410 (0.1%)
1	C	0.66	4/2511 (0.2%)	0.68	0/3421
1	E	0.63	1/2511 (0.0%)	0.69	1/3421 (0.0%)
2	B	0.76	2/1423 (0.1%)	0.71	2/1912 (0.1%)
2	D	0.72	0/1414	0.79	0/1894
2	F	0.70	2/1423 (0.1%)	0.74	0/1912
All	All	0.67	11/11784 (0.1%)	0.71	5/15970 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	58	LYS	CE-NZ	13.52	1.82	1.49
1	C	9	SER	CB-OG	9.31	1.54	1.42
2	B	58	LYS	CD-CE	7.72	1.70	1.51
1	E	158	GLY	C-O	7.07	1.34	1.23
1	A	321	ARG	CZ-NH2	7.06	1.42	1.33
1	C	158	GLY	C-O	5.64	1.32	1.23
2	F	57	GLU	CG-CD	5.47	1.60	1.51
2	F	132	GLU	CG-CD	-5.30	1.44	1.51
1	C	14	CYS	CB-SG	-5.24	1.73	1.81
1	A	238	LYS	CD-CE	5.10	1.64	1.51
1	C	208	ARG	CZ-NH2	5.04	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	NE-CZ-NH1	-7.90	116.35	120.30
2	B	58	LYS	CD-CE-NZ	-7.53	94.38	111.70
1	E	321	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	A	321	ARG	NE-CZ-NH2	6.22	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	LEU	CB-CG-CD2	-5.71	101.29	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2446	0	2397	33	0
1	C	2455	0	2410	55	0
1	E	2455	0	2410	41	0
2	B	1399	0	1319	26	0
2	D	1390	0	1319	34	0
2	F	1399	0	1319	24	0
3	D	24	0	27	2	0
3	F	12	0	12	1	0
All	All	11580	0	11213	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LYS:CE	2:B:58:LYS:NZ	1.82	1.39
1:C:208:ARG:NH2	1:C:238:LYS:HE3	1.58	1.15
1:C:208:ARG:HH22	1:C:238:LYS:HE3	1.09	1.01
2:D:128:GLU:HG3	2:D:170:ARG:HH11	1.33	0.94
1:C:216:ASN:ND2	1:E:212:THR:OG1	2.01	0.94
1:C:99:PRO:CD	1:C:226:LEU:HD12	2.00	0.90
1:E:63:ASP:OD1	1:E:92:LYS:HG3	1.74	0.87
2:D:30:GLU:OE1	2:D:146:ASN:CG	2.14	0.84
1:C:182:ILE:HD11	1:C:215:PRO:HD3	1.61	0.81
1:C:99:PRO:HD3	1:C:226:LEU:HD12	1.63	0.80
1:C:221:PRO:O	1:C:229:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:HG2	2:B:134:GLY:H	1.46	0.78
2:D:128:GLU:HG3	2:D:170:ARG:NH1	2.00	0.76
1:E:283:THR:OG1	1:E:286:GLY:O	2.05	0.74
1:E:99:PRO:CD	1:E:226:LEU:HD12	2.19	0.73
1:E:230:ILE:HD13	1:E:252:ILE:HG13	1.70	0.73
1:E:99:PRO:HD3	1:E:226:LEU:HD12	1.72	0.70
1:A:98:TYR:CD2	1:A:99:PRO:HD2	2.27	0.69
1:A:283:THR:OG1	1:A:286:GLY:O	2.09	0.69
3:F:173:EYK:HAC	3:F:173:EYK:OAE	1.93	0.69
1:E:309:VAL:HG13	1:E:311:GLN:OE1	1.93	0.68
1:C:77:ASP:O	1:C:80:GLN:HG3	1.95	0.66
2:B:58:LYS:NZ	2:B:58:LYS:CD	2.59	0.66
2:B:132:GLU:HG2	2:B:134:GLY:N	2.12	0.65
2:D:30:GLU:OE1	2:D:146:ASN:ND2	2.30	0.65
1:C:141:ARG:NH1	1:C:147:PHE:O	2.31	0.63
2:B:150:GLU:HG2	2:B:153:ARG:NH2	2.12	0.63
1:C:99:PRO:HD2	1:C:226:LEU:HD12	1.79	0.63
2:B:132:GLU:CG	2:B:134:GLY:H	2.12	0.63
1:C:307:LYS:HE3	2:D:60:ASN:HD21	1.64	0.63
1:A:182:ILE:HD13	1:A:213:ILE:HG22	1.82	0.62
2:D:5:ALA:O	2:D:10:ILE:HB	2.01	0.61
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.65	0.61
1:C:275:ASP:OD2	1:C:276:THR:N	2.33	0.61
1:C:222:TRP:CZ2	1:C:225:GLY:HA2	2.37	0.60
1:C:77:ASP:OD1	1:C:141:ARG:NH2	2.35	0.59
2:B:150:GLU:HG2	2:B:153:ARG:HH22	1.67	0.59
1:C:216:ASN:CG	1:E:212:THR:OG1	2.41	0.59
1:A:158:GLY:O	1:A:159:SER:HB3	2.03	0.59
2:B:56:ILE:HG22	2:B:56:ILE:O	2.03	0.59
2:F:54:ARG:O	2:F:57:GLU:HG2	2.03	0.59
2:D:168:ASN:HA	2:D:172:GLN:OE1	2.03	0.58
2:F:74:GLU:HG3	2:F:78:GLN:NE2	2.18	0.58
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.38	0.58
1:C:90:ARG:NH1	1:C:274:ILE:HD12	2.18	0.58
1:C:208:ARG:CZ	1:C:238:LYS:HG3	2.35	0.57
1:C:325:GLU:O	1:C:326:LYS:HB3	2.03	0.57
1:C:84:TRP:HZ3	1:C:118:LEU:HG	1.69	0.57
1:A:97:CYS:O	1:A:224:ARG:NH1	2.30	0.57
1:E:213:ILE:HD12	1:E:213:ILE:N	2.19	0.57
3:D:174:EYK:OAE	3:D:174:EYK:HAC	2.04	0.56
1:A:77:ASP:O	1:A:80:GLN:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:TRP:HZ3	1:E:118:LEU:HG	1.72	0.55
2:B:168:ASN:ND2	2:B:172:GLN:CG	2.70	0.55
2:D:2:LEU:HB3	2:F:3:PHE:CZ	2.40	0.55
2:D:52:LEU:CD1	2:D:56:ILE:HD12	2.37	0.55
1:C:185:PRO:HG2	1:C:191:GLN:OE1	2.07	0.55
1:A:129:GLY:HA3	1:A:162:PRO:HG3	1.88	0.55
3:D:173:EYK:HAC	3:D:173:EYK:OAE	2.06	0.54
2:F:171:PHE:O	2:F:172:GLN:HB2	2.07	0.54
2:B:125:GLN:OE1	2:B:155:GLY:HA2	2.08	0.54
1:A:207:ARG:HG2	1:E:223:VAL:HG22	1.90	0.54
1:E:77:ASP:OD1	1:E:141:ARG:NH2	2.41	0.54
1:E:23:GLY:HA3	1:E:35:GLU:OE2	2.08	0.54
1:E:77:ASP:O	1:E:80:GLN:HG3	2.08	0.54
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.91	0.53
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.90	0.53
1:C:309:VAL:HG13	1:C:311:GLN:OE1	2.09	0.53
1:A:81:ASN:ND2	1:A:120:PHE:H	2.06	0.53
1:A:81:ASN:HD21	1:A:120:PHE:H	1.56	0.52
1:A:249:GLY:O	1:A:250:ASN:HB2	2.08	0.52
1:A:186:SER:HA	1:A:218:GLY:O	2.09	0.52
1:C:213:ILE:HG12	1:C:233:TYR:CZ	2.44	0.52
1:A:31:ASP:OD2	1:A:34:ILE:HD12	2.10	0.52
2:D:120:GLU:CD	2:D:123:ARG:HH22	2.13	0.52
1:A:84:TRP:CZ3	1:A:118:LEU:HG	2.44	0.52
2:D:52:LEU:HD11	2:D:56:ILE:CD1	2.40	0.52
1:A:52:CYS:HB3	1:A:277:CYS:O	2.10	0.51
1:E:51:ILE:HG23	1:E:282:ILE:HD12	1.92	0.51
1:C:307:LYS:CE	2:D:60:ASN:HD21	2.21	0.51
1:E:307:LYS:NZ	2:F:60:ASN:OD1	2.29	0.51
1:C:51:ILE:HG23	1:C:282:ILE:HD12	1.91	0.51
1:C:163:VAL:O	1:C:163:VAL:HG23	2.11	0.51
1:C:99:PRO:HD2	1:C:226:LEU:CD1	2.40	0.51
1:C:208:ARG:NH2	1:C:238:LYS:CE	2.52	0.51
2:F:150:GLU:OE1	2:F:153:ARG:NH2	2.44	0.50
1:A:98:TYR:CZ	1:A:226:LEU:HD13	2.47	0.50
2:D:56:ILE:O	2:D:56:ILE:HG22	2.11	0.50
1:C:90:ARG:HH12	1:C:274:ILE:HD12	1.77	0.50
1:C:216:ASN:ND2	1:E:203:THR:OG1	2.45	0.50
2:F:54:ARG:HA	2:F:57:GLU:CD	2.31	0.50
1:C:98:TYR:CD2	1:C:99:PRO:HD2	2.46	0.50
2:D:132:GLU:CD	2:F:124:ARG:HE	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:THR:OG1	1:C:319:GLY:HA3	2.12	0.49
2:F:119:PHE:HZ	2:F:132:GLU:CG	2.25	0.49
1:C:127:TRP:CZ3	1:C:166:VAL:HG21	2.47	0.49
2:D:53:ASN:O	2:D:57:GLU:HB2	2.12	0.49
2:D:132:GLU:OE2	2:F:124:ARG:NE	2.42	0.49
1:A:133:ASN:OD1	1:A:255:ARG:NH1	2.46	0.49
1:C:163:VAL:O	1:C:163:VAL:CG2	2.61	0.49
1:E:98:TYR:CD2	1:E:99:PRO:HD2	2.48	0.49
1:C:26:VAL:HG22	1:C:34:ILE:O	2.12	0.48
2:B:51:LYS:HE3	2:B:107:THR:OG1	2.13	0.48
2:B:27:GLN:HB2	2:B:32:THR:HG22	1.96	0.48
1:C:310:LYS:HE3	2:D:90:ASP:OD2	2.13	0.48
1:C:28:THR:HB	2:D:105:GLN:OE1	2.13	0.48
2:B:142:HIS:CD2	2:B:162:TYR:HB3	2.49	0.48
1:E:151:LEU:O	1:E:255:ARG:NH2	2.46	0.48
2:F:25:ARG:HG3	2:F:34:GLN:HG3	1.96	0.48
2:F:74:GLU:HG3	2:F:78:GLN:HE21	1.77	0.48
2:D:2:LEU:HB3	2:F:3:PHE:HZ	1.79	0.47
2:B:168:ASN:ND2	2:B:172:GLN:HG3	2.29	0.47
2:F:54:ARG:HA	2:F:57:GLU:OE2	2.14	0.47
1:A:89:GLU:OE2	1:A:109:ARG:NH2	2.48	0.47
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.96	0.47
2:D:132:GLU:HG2	2:D:134:GLY:H	1.80	0.47
2:F:17:MET:HE2	2:F:20:GLY:O	2.15	0.47
1:C:320:MET:HG3	1:C:321:ARG:O	2.15	0.47
2:B:139:LYS:HE2	2:B:141:TYR:CE2	2.49	0.47
2:D:56:ILE:O	2:D:56:ILE:CG2	2.63	0.47
1:C:216:ASN:ND2	1:E:212:THR:CB	2.78	0.46
1:A:26:VAL:HG13	2:B:104:ASN:ND2	2.31	0.46
2:D:2:LEU:O	2:F:113:SER:OG	2.32	0.46
1:C:99:PRO:HB2	1:C:229:ARG:HD3	1.97	0.46
1:C:176:LYS:HE2	1:C:257:TYR:CE2	2.51	0.46
1:C:208:ARG:HH22	1:C:238:LYS:CE	2.00	0.46
2:B:2:LEU:HB3	2:D:3:PHE:HZ	1.82	0.45
2:B:2:LEU:HB3	2:D:3:PHE:CZ	2.51	0.45
2:B:58:LYS:H	2:B:58:LYS:HG3	1.62	0.45
2:B:139:LYS:HE2	2:B:141:TYR:CZ	2.52	0.45
1:E:87:PHE:O	1:E:267:ILE:HG13	2.17	0.45
2:D:139:LYS:HD3	2:D:141:TYR:CZ	2.51	0.45
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.52	0.45
1:E:212:THR:C	1:E:213:ILE:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:GLU:HG3	2:F:170:ARG:HD2	1.98	0.45
1:E:89:GLU:HG3	1:E:267:ILE:HD11	1.97	0.45
1:A:291:ASP:O	2:B:56:ILE:HG23	2.16	0.44
1:E:84:TRP:CZ3	1:E:118:LEU:HG	2.52	0.44
2:F:56:ILE:HG22	2:F:56:ILE:O	2.15	0.44
1:C:127:TRP:CH2	1:C:166:VAL:HG21	2.52	0.44
1:C:325:GLU:O	1:C:326:LYS:CB	2.66	0.44
2:D:125:GLN:OE1	2:D:155:GLY:HA2	2.17	0.44
2:F:17:MET:HE2	2:F:17:MET:HB3	1.78	0.44
1:C:121:ILE:HD12	1:C:257:TYR:CE1	2.52	0.44
1:C:274:ILE:HG22	1:C:275:ASP:N	2.33	0.44
1:E:31:ASP:OD2	1:E:34:ILE:HD12	2.18	0.43
2:B:106:HIS:CE1	2:B:110:LEU:HD23	2.53	0.43
1:E:119:GLU:OE1	1:E:261:ARG:NH2	2.50	0.43
2:D:135:ASN:OD1	2:D:135:ASN:N	2.52	0.43
2:F:171:PHE:O	2:F:172:GLN:CB	2.65	0.43
1:C:15:LEU:HD22	2:D:119:PHE:HA	2.00	0.43
1:E:97:CYS:O	1:E:224:ARG:NH1	2.45	0.43
1:E:176:LYS:HE2	1:E:257:TYR:CE2	2.53	0.43
1:A:188:ASN:HA	1:A:191:GLN:HB3	2.00	0.43
2:D:30:GLU:OE1	2:D:146:ASN:CB	2.67	0.43
1:E:15:LEU:HD22	2:F:119:PHE:HA	2.00	0.43
1:E:310:LYS:HB2	1:E:310:LYS:HE3	1.79	0.43
1:A:161:TYR:HA	1:A:162:PRO:HD2	1.86	0.43
1:C:84:TRP:CZ3	1:C:118:LEU:HG	2.51	0.43
1:A:163:VAL:HG22	1:A:248:ASN:HB3	2.01	0.43
1:A:57:ARG:HD3	1:A:83:THR:O	2.19	0.42
2:B:131:GLU:OE1	2:D:127:ARG:NH2	2.50	0.42
1:C:98:TYR:CZ	1:C:226:LEU:HD13	2.53	0.42
1:E:301:THR:HB	1:E:305:CYS:SG	2.59	0.42
1:E:89:GLU:OE2	1:E:109:ARG:NH2	2.51	0.42
1:C:67:ILE:HD12	1:C:108:LEU:HD23	2.01	0.42
1:E:213:ILE:HG12	1:E:233:TYR:CZ	2.54	0.42
1:E:29:ILE:HD13	1:E:29:ILE:HA	1.92	0.42
1:E:71:LEU:O	1:E:148:PHE:HB3	2.19	0.42
1:A:97:CYS:HA	1:A:139:CYS:HB2	2.02	0.41
1:A:213:ILE:HG12	1:A:233:TYR:CZ	2.55	0.41
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.55	0.41
1:C:290:ASN:HB2	2:D:59:THR:HG21	2.03	0.41
2:F:163:ARG:O	2:F:167:LEU:HG	2.20	0.41
1:A:244:VAL:HG23	1:E:221:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:CD	2:D:124:ARG:HE	2.23	0.41
1:C:90:ARG:NH1	1:C:274:ILE:CD1	2.82	0.41
1:C:221:PRO:HG2	1:E:206:THR:C	2.41	0.41
1:A:62:ILE:HG22	1:A:63:ASP:N	2.36	0.41
1:C:99:PRO:CD	1:C:226:LEU:CD1	2.85	0.40
2:D:132:GLU:CG	2:D:134:GLY:H	2.33	0.40
1:E:15:LEU:HD23	2:F:118:LEU:HG	2.02	0.40
2:F:128:GLU:OE1	2:F:170:ARG:NH1	2.53	0.40
2:B:170:ARG:HG2	2:B:171:PHE:CE1	2.56	0.40
1:C:97:CYS:SG	1:C:98:TYR:N	2.90	0.40
1:A:170:ASN:HA	1:A:176:LYS:NZ	2.36	0.40
1:E:213:ILE:N	1:E:213:ILE:CD1	2.83	0.40
2:D:14:TRP:HE3	2:D:17:MET:HE3	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/321 (98%)	304 (96%)	10 (3%)	1 (0%)	41	72
1	C	316/321 (98%)	296 (94%)	18 (6%)	2 (1%)	25	56
1	E	316/321 (98%)	301 (95%)	14 (4%)	1 (0%)	41	72
2	B	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
2	D	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
2	F	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
All	All	1457/1479 (98%)	1390 (95%)	63 (4%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	E	62	ILE
1	C	62	ILE
1	C	143	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/283 (99%)	275 (99%)	4 (1%)	67	90
1	C	280/283 (99%)	276 (99%)	4 (1%)	67	90
1	E	280/283 (99%)	276 (99%)	4 (1%)	67	90
2	B	147/147 (100%)	145 (99%)	2 (1%)	67	90
2	D	147/147 (100%)	143 (97%)	4 (3%)	44	78
2	F	147/147 (100%)	146 (99%)	1 (1%)	84	95
All	All	1280/1290 (99%)	1261 (98%)	19 (2%)	65	89

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	141	ARG
1	A	261	ARG
1	A	321	ARG
2	B	57	GLU
2	B	58	LYS
1	C	18	HIS
1	C	141	ARG
1	C	265	SER
1	C	312	ASN
2	D	54	ARG
2	D	128	GLU
2	D	150	GLU
2	D	160	ASP
1	E	18	HIS

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Mol	Chain	Res	Type
1	E	215	PRO
1	E	222	TRP
1	E	224	ARG
2	F	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	80	GLN
1	A	81	ASN
2	B	168	ASN
1	C	38	ASN
1	C	216	ASN
2	D	60	ASN
2	D	65	GLN
1	E	38	ASN
1	E	165	ASN
1	E	246	ASN
2	F	78	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EYK	D	174	-	12,12,12	1.38	2 (16%)	18,18,18	2.60	7 (38%)
3	EYK	F	173	-	12,12,12	1.11	1 (8%)	18,18,18	2.27	6 (33%)
3	EYK	D	173	-	12,12,12	1.12	1 (8%)	18,18,18	2.31	8 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EYK	D	174	-	-	0/6/6/6	0/1/1/1
3	EYK	F	173	-	-	3/6/6/6	0/1/1/1
3	EYK	D	173	-	-	0/6/6/6	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	174	EYK	CAH-CAI	3.66	1.44	1.39
3	D	173	EYK	CAH-CAI	2.49	1.42	1.39
3	F	173	EYK	CAH-CAI	2.38	1.42	1.39
3	D	174	EYK	CAG-CAJ	2.06	1.43	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	174	EYK	CAL-CAK-CAJ	-6.79	118.07	122.20
3	D	173	EYK	CAL-CAK-CAJ	-4.85	119.25	122.20
3	F	173	EYK	CAL-CAK-CAJ	-4.57	119.42	122.20
3	F	173	EYK	CAA-CAL-CAK	4.42	119.28	110.87
3	D	174	EYK	CAA-CAL-CAK	4.10	118.67	110.87
3	D	173	EYK	CAG-CAJ-CAK	4.09	124.46	120.46
3	F	173	EYK	CAC-CAL-CAA	-3.79	97.09	108.36
3	D	173	EYK	CAA-CAL-CAK	3.76	118.03	110.87
3	D	174	EYK	CAC-CAL-CAA	-3.75	97.19	108.36
3	F	173	EYK	CAG-CAF-CAI	-3.67	116.00	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	174	EYK	CAG-CAF-CAI	-3.42	116.26	119.88
3	D	173	EYK	CAB-CAL-CAK	-3.16	104.85	110.87
3	D	174	EYK	CAG-CAJ-CAK	2.82	123.22	120.46
3	D	173	EYK	CAC-CAL-CAA	-2.71	100.29	108.36
3	D	173	EYK	CAG-CAF-CAI	-2.68	117.04	119.88
3	D	174	EYK	CAH-CAK-CAL	2.65	126.74	120.19
3	F	173	EYK	CAG-CAJ-CAK	2.61	123.01	120.46
3	F	173	EYK	CAH-CAK-CAL	2.24	125.71	120.19
3	D	173	EYK	CAC-CAL-CAK	2.20	115.06	110.87
3	D	173	EYK	CAF-CAI-CAH	2.13	122.53	120.19
3	D	174	EYK	CAB-CAL-CAK	-2.08	106.90	110.87

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	173	EYK	CAJ-CAK-CAL-CAA
3	F	173	EYK	CAJ-CAK-CAL-CAB
3	F	173	EYK	CAH-CAK-CAL-CAA

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	174	EYK	1	0
3	F	173	EYK	1	0
3	D	173	EYK	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	317/321 (98%)	-0.25	9 (2%)	53	43	40, 56, 81, 89	0
1	C	318/321 (99%)	-0.13	9 (2%)	53	43	41, 61, 81, 91	0
1	E	318/321 (99%)	-0.28	6 (1%)	66	59	38, 54, 69, 84	0
2	B	172/172 (100%)	-0.32	6 (3%)	44	34	36, 57, 79, 91	0
2	D	172/172 (100%)	-0.44	3 (1%)	70	63	35, 51, 70, 90	0
2	F	172/172 (100%)	-0.48	3 (1%)	70	63	36, 52, 70, 89	0
All	All	1469/1479 (99%)	-0.29	36 (2%)	57	47	35, 55, 79, 91	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	143	PRO	4.2
1	C	142	GLY	4.1
2	F	58	LYS	3.9
1	A	143	PRO	3.9
1	A	222	TRP	3.8
2	B	58	LYS	3.5
2	D	58	LYS	3.4
2	B	18	ILE	3.4
1	A	22	ASN	3.3
2	D	57	GLU	3.1
1	C	208	ARG	3.1
1	C	222	TRP	3.0
1	E	22	ASN	2.9
2	B	29	SER	2.9
1	E	143	PRO	2.8
1	A	189	GLN	2.7
1	E	326	LYS	2.7
1	E	222	TRP	2.6
2	B	71	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	2.6
1	A	173	ASN	2.6
2	F	60	ASN	2.4
1	E	144	GLY	2.2
2	B	32	THR	2.2
1	C	158	GLY	2.2
1	A	21	PRO	2.2
2	D	18	ILE	2.2
2	F	18	ILE	2.1
1	A	144	GLY	2.1
1	C	193	SER	2.1
1	E	142	GLY	2.1
1	C	189	GLN	2.0
1	C	144	GLY	2.0
1	A	325	GLU	2.0
1	C	159	SER	2.0
2	B	172	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EYK	D	173	12/12	0.89	0.27	62,72,77,80	0
3	EYK	D	174	12/12	0.91	0.24	54,62,66,66	0
3	EYK	F	173	12/12	0.92	0.27	58,67,70,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.